D-Galactitol

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 1.66

Global applicability domain: Outside

Local applicability domain index: 2.05e-01

Confidence level: 7.19e-01

Nearest Neighbors from the Training Set

Image not found
Pentaerythritol
Measured: 1.26
Predicted: 1.25

Image not found
Tris(2-hydroxyethyl) isocyanurate
Measured: 1.58
Predicted: 1.61

Image not found
Cyanuric acid
Measured: 5.01e-01
Predicted: 1.72

Image not found
Melamine
Measured: 3.80
Predicted: 2.45

Image not found
Triethanolamine
Measured: 3.89
Predicted: 2.97